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Modelling the effect of sampling methods on detection tests for powdered products

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ABSTRACT

Grab sampling is often a convenient and cost effective way to sample bulk food materials, such as milk powder. On the other hand, modern auto-samplers can sample very small increments directly from the production process and they can be set to collect primary increments systematically. While the quantity of sampled bulk material is important, it is also necessary to consider the impact of sampling on quantitative risk assessment. When grab samples are drawn, the principle of randomisation is only partially met because of the inability to draw small primary increments at random. Food contamination (microbiological or otherwise) does not occur uniformly, and is often patchy or heterogeneous within a batch. Hence, even random sampling of primary increments does not amount to random sampling of pathogens or contaminants. As a consequence, the consumer's risk is underestimated under the holistic assumption of complete randomisation. In this theoretical study, a correlation parameter is introduced to allow for lack of independence in the presence and absence of contamination, and then the effect of the various sampling methods on the consumer's risk is examined. The main conclusion from this study is that grab sampling can increase the consumer's risk by as much as 50% and hence additional sampling is necessary when grab samples are used for lot disposition when compared to directly sampling the product from the process, which can be done using auto-samplers.

1. Introduction

The International Commission on Microbiological Specifications for Foods (ICMSF) has published recommendations, guidelines and tools for microbiological sampling inspection over the years; see ICMSF (1986), ICMSF (2002), ICMSF (2009) and ICMSF (2011). Similar guidelines, policies, recommendations and standards relating to food safety, and particularly on the use of inspection plans for the food trade, have been given by the Codex Alimentarius; see CAC (1997) and CAC (2004). The Food and Agriculture Organization of the United Nations (FAO) and the World Health Organization (WHO) regularly promote joint expert meetings and publish recommendations on sampling plans for different micro-organisms of interest; see FAO/WHO (2016).

Food products are typically bulk in nature, and hence random sampling of food products is difficult unless they are packaged in small volumes. If the population of interest consists of N discrete items, a simple random sample of size n can be easily drawn using a random number generation tool. Even when food is packaged, random selection of packages does not amount to random selection of primary units or increments unless the quality or safety characteristic of interest is completely homogeneous. As the characteristics are microbial in nature, they cannot be randomly sampled at all. However, microbiological and other food quality sampling inspection plans are typically evaluated under the holistic assumption of random sampling. The bias caused by the non-random sampling method can be large. This bias can increase the probabilities of false negative cases and also reduce the probability of false positive and vice versa. In other words, the designated consumer's and producer's risks under the chosen sampling inspection plan may be exceeded. Hence it is important to examine the violations of random sampling assumption for risk assessment and management.

In the industrial production of powdered food products such as milk powder, usually robotic or automatic samplers are employed to sample very small quantities, such as 1g, from the production process. Auto-samplers are often set to sample systematically, such that a total quantity such as 5kg can be accumulated to provide an overall representation of the product quality. Even though auto samplers can be programmed to perform random sampling, the common practice is to set them to sample systematically, for example every 5 min.

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The term *grab sampling* refers to the draw of a specified quantity of material, and this sampling procedure is common not only for packaged bulk products but also the sampling of water, soil etc in environmental, agricultural, and geophysical studies. A grab sample is basically a "block" of successive or clustered unit amounts of the material drawn from flowing production process material at a particular time point or drawn as a block amount from a packaged material. Each grab sample can be viewed as a block of several primary increments. Even though grab samples can be selected both randomly and systematically, the principle of randomisation does not extend to the selection of primary increments. In other words, there is bound to be within grab sample variability and such variation is unlikely to be random. There is a scarcity of literature dealing with grab sampling theory. Gy's Theory Of Sampling (TOS) literature is critical of grab sampling methods, because it ignores the irreducible fundamental error, and other material sub-sampling errors in the test sample preparation; see Gy (1979), Pitard (1993) and Minkkinen and Esbensen (2009). The TOS literature warns that the grab sampling is the worst performing approach among all of the mass reduction approaches; see Minkkinen and Esbensen (2009). Mathematical modelling of the grab sampling method is scarce in the TOS literature because comparison is largely done using empirical methods.

When food products are sampled for regulatory and export inspections, the underlying product is in packaged form. Hence most samples drawn from the batch must be treated as random grab samples. On the other hand, the producer's quality and safety inspection schemes are based on grab or auto-samples drawn directly from the production process. Even though random grab sampling from the flow of the products over time is desirable, regulatory inspection cannot rely on the producer's samples due to legal and consumer protection issues. The main aim of this article is to quantify the inefficiency of the grab sampling method when compared to systematic auto sampling and how to possibly compensate for this inefficiency with higher sample sizes.

In Section 2, an underlying mathematical formulation of the production process incorporate sequential dependence via the primary increments is given. Four possible methods of sampling are then described. The comparison of four sampling approaches based on presence - absence testing is discussed in Section 3. Finally, additional operating characteristic properties are studied in Section 4.

2. Methodology

Most powdered food products are produced in large volumes, such as 20 tons, through a single production run. Even though the produced material is continuous and not discrete like nuts and bolts, we may define a very small quantity or primary increment such as 1g and then conceptually discretise the production volume (say, 20 tons) into a very long chain made of 1g primary increments. This approach of discretising bulk material production was employed in Govindaraju et al. (2017). Let the bulk material production process be modelled as a series $\{X_1, X_2, \ldots, X_N\}$ where $N = \text{int}(M/s)$ for known total production quantity M and a small primary incremental amount s. Usually, N is a very large number (in the billions) for food production processes but can be in millions of primary increments for kilogram scale pharmaceutical production processes.

Let $X_j = 1$ or 0 depending on the presence or absence of contamination. By our construction, the X_j's are serially correlated. Contamination is often spotty even when the main quality characteristics of the product (such as percentage protein and fat) are relatively homogeneous. We assume that the bulk material production process can be modelled as a one step two-state Markov chain with the transition matrix,

$$\mathbf{P} = \begin{matrix} \\ 0 \\ 1 \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 1-a & a \\ b & 1-b \end{bmatrix} \end{matrix} \tag{1}$$

Table 1
Glossary of symbols and abbreviations.

M	total production quantity
S	primary incremental amount
N	length of the production in primary increments
X_i	contamination status of the i^{th} primary increment
a	probability of contamination of the primary increment when it is absent in the previous increment
b	probability of contamination of the primary increment when it is present in the previous increment
c	acceptance number
p	limiting fraction or proportion of contaminated increments
d	serial correlation of contamination between the primary increments
d_g	serial correlation of contamination between blocks or grab samples
k	sampling interval of the systematic sampling procedure
f	sampling frequency of the systematic sampling procedure
D	serial correlation between the systematically sampled primary increments
D_g	serial correlation between the systematically drawn grab samples
$\mathbf{P}$	transition matrix for X_i
$\mathbf{P_k}$	transition matrix for systematic primary increment sampling of X_i
$\mathbf{P_{G_k}}$	transition matrix for systematic grab sampling of X_i
P_{D}	probability of detection
P_{ND}	probability of non-detection
r	grab sample size or the number of primary increments in a grab sample
t	number of grab samples
n	number of primary increments in selected samples ($n = rt$ for grab samples)
y_i	i^{th} primary increment
$y_{i(j)}$	j^{th} primary increment in i^{th} block (grab sample)
p_d	probability of detection in any block (grab sample)
p_{nd}	probability of non-detection in any block (grab sample)
a^*	probability of contaminated block given that the previous block is not contaminated
b^*	probability of uncontaminated block given that the previous block is contaminated
μ	location parameter (mean log) of the Lognormal and Poisson-lognormal distributions on the log10 scale
σ	standard deviation of the lognormal and Poisson-lognormal distributions on the log10 scale (default value 0.8)
λ	arithmetic mean of the cell counts
K	dispersion parameter of the Poisson gamma distribution
m	microbiological limit
$\lceil f \rceil$	ceiling or least integer function giving the smallest integer that is not smaller than f
TOS	Theory Of Sampling
ND	Non-Detect
D	Detect
OC	Operating Characteristic
OQ	Outgoing Quality
AOQ	Average Outgoing Quality
AOQL	Average Outgoing Quality Limit

$(0 \le a, b \le 1)$, where a is the probability of contamination in the primary increment when it is absent in the previous increment. The difference $d = 1 - a - b$ is interpreted as the *serial correlation* of the X_j's in the statistics literature; see Bebbington and Lai (1998), Govindaraju et al. (2017). The limiting fraction of contaminated increments $P(X_j = 1) = p$ is given by $a/(a + b)$. An alternative parameterization of $\mathbf{P}$ in terms of p and d is given by,

$$P = \begin{matrix} \\ 0 \\ 1 \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 1-(1-d)p & (1-d)p \\ (1-d)(1-p) & p+(1-p)d \end{bmatrix} \end{matrix}, \text{ see Govindaraju et al. (2017).} \tag{2}$$

Detection of contamination not only depends on the prevalence p but also relies on the method of sampling. We consider four different scenarios. The first one is the direct simple random sampling of primary increments, while the second one is systematic sampling of primary increments. The other two methods are, respectively, random and systematic sampling of grab samples instead of primary increments. Table 1

gives the glossary of various notations and terminology employed for these four methods of sampling for contamination detection.

2.1. Simple random sampling of primary increments

Even though it is in practice very difficult to perform, we consider the simple random sampling of primary increments for comparative risk evaluation purposes. Under simple random sampling, serial correlation can be ignored and only the limiting fraction matters. Hence, if n primary increments are selected at random for a presence-absence type test on each sampled increment, the detection probability under the simple random sampling method is given by

$$P_D = 1 - (1-p)^n \tag{3}$$

2.2. Systematic sampling of primary increments

Systematic sampling of primary increments can be implemented using a high-tech robotic auto-sampler. Let $k = \lceil 1/f \rceil$ where $\lceil 1/f \rceil$ is the ceiling or least integer function for upward rounding of $1/f$ to an integer, and f is the sampling frequency of the systematic sampling procedure. If one primary increment is selected for every k^{th} increment produced, the two-state Markov chain model described above applies. Systematic sampling from this process model is discussed in Vellaisamy and Sankar (2001) and Govindaraju et al. (2017). Let $\{y_1, y_{k+1}, y_{2k+1}, \cdots, y_{(n-1)k+1}\}$ for some integer $k \geq 1$, be the systematic selected auto-samples of n primary increments. Then the one step transition matrix for the two-state Markov chain of the presence and absence of contamination in selected auto-samples is given by,

$$\mathbf{P_k} = \begin{matrix} \\ 0 \\ 1 \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 1-A & A \\ B & 1-B \end{bmatrix} \end{matrix} = \begin{matrix} \\ 0 \\ 1 \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 1-p(1-d^k) & p(1-d^k) \\ (1-p)(1-d^k) & p+(1-p)d^k \end{bmatrix} \end{matrix} \tag{4}$$

where $A = p(1-d^k)$, and $B = (1-p)(1-d^k)$; see Govindaraju et al. (2017). The steady state probabilities of $\mathbf{P_k}$ are the same as that of the original Markov chain $\mathbf{P}$ in Eq. (2). The serial correlation between the auto samples, D, is equal to $D = 1 - A - B = d^k$. Following Vellaisamy and Sankar (2001), the probability of non-detection in two consecutive systematic auto-samples is given by $(1-A)(1-p)$ and hence the probability of non-detection in a set of systematic auto-samples becomes

$$P_{\text{ND}} = (1-p)(1-A)^{n-1} = (1-p)\left(1-p\left(1-d^k\right)\right)^{n-1} \tag{5}$$

Alternatively we can express this as the probability of detection

$$P_{\text{D}} = 1 - (1-p)\left[\left(1-p\left(1-d^k\right)\right)\right]^{n-1} \tag{6}$$

where $k = \lceil N/n \rceil$; see Appendix A for further details.

2.3. Random selection of grab samples

We now consider random selection of grab samples, which are basically blocks of primary increments. Each block has two possible outcomes ND (non-detect) or D (detect) depending on whether a contaminated primary increment is absent or present in a particular block. The state space {ND, D} also becomes a two-state Markov chain, and the serial correlation between blocks is given as $d_g = [dp(1-p(1-d))^{r-1}]/p_d$ where r is the number of consecutive primary increments which form the grab sample (see Appendix A).

Let the i^{th} block be $\{y_{i(1)}, y_{i(2)}, \ldots, y_{i(r)}\}$. The probability of non-detection for the i^{th} grab sample is given by

$$\begin{aligned} &P(\text{non}-\text{detection in block } i) = P(y_{i(1)} = 0, y_{i(2)} = 0, \ldots, y_{i(r)=0}) = \\ &P(y_{i(1)} = 0)P(y_{i(2)} = 0 | y_{i(1)} = 0)P(y_{i(3)} = 0 | y_{i(2)} = 0, y_{i(1)} = 0)\cdots \\ &P(y_{i(r)} = 0 | y_{i(1)} = 0, y_{i(2)} = 0 \ldots y_{i(r-1)} = 0) \end{aligned} \tag{7}$$

This probability can be simplified as

$$p_{nd} = (1-p)(1-p(1-d))^{r-1} \tag{8}$$

which is valid for any block i, of size r, and hence the probability of detection in any block is given by

$$p_d = 1 - (1-p)(1-p(1-d))^{r-1} \tag{9}$$

Under random grabsampling, serial correlation between blocks can again be ignored, and hence the underlying Markov process converges to a series of independent Bernoulli trials. Consequently, if t grab samples are randomly selected and tested, the detection probability becomes

$$P_{\text{D}} = 1 - (1-p_d)^t \tag{10}$$

2.4. Systematic selection of grab samples

Systematic selection of grab samples is difficult with packaged food product. Only the packaged unit of product can be sampled systematically and hence sub-sampling becomes necessary to obtain the regular analytical test sample amount, such as 10g. On the other hand, time oriented systematic selection of grab samples can be easily done using robotic samplers. For example, the auto samplers can be set to sample 10g of samples every half an hour instead of selecting a very small amount such as 1g at every 3 min. Under this sampling method, grab samples (blocks) are taken systematically with sampling frequency f from the production process in a given period; where $f = rt/N$. Let $k = \lceil 1/f \rceil$ be the systematic grab sampling interval, which means every k^{th} lump of primary increments (block) is periodically collected from the production process. The results given in Vellaisamy and Sankar (2001) and Govindaraju et al. (2017) are valid for systematic primary increments selection, but these results can be modified for systematic block selection, substituting for p with p_d and d with d_g. The resulting transition matrix for the one-step two-state Markov chain describing the systematic selection of grab samples is given by,

$$\mathbf{P_{G_k}} = \begin{matrix} \\ \text{ND} \\ \text{D} \end{matrix} \begin{matrix} \begin{matrix} \text{ND} & \text{D} \end{matrix} \\ \begin{bmatrix} 1-E & E \\ F & 1-F \end{bmatrix} \end{matrix} \tag{11}$$

where $E = p_d(1-d_g^k)$, and $F = (1-p_d)(1-d_g^k)$. The vector of steady state probabilities is equal to $[1-p_d, p_d]$ which is different from the vector $[1-p, p]$ valid for the original series X's. Also, the serial correlation between the systematic grab samples becomes $D_g = 1 - E - F = d_g^k$. The probability of non-detection with the t systematic grab samples is then given by,

$$P_{\text{ND}} = (1-p_d)\left[\left(1-p_d\left(1-d_g^k\right)\right)\right]^{t-1} \tag{12}$$

Hence the detection probability with the t selected grab samples is

$$P_{\text{D}} = 1 - (1-p_d)\left[\left(1-p_d\left(1-d_g^k\right)\right)\right]^{t-1} \tag{13}$$

where $k = \lceil N/rt \rceil$. If $r = 1$ and $t = n$ then $\mathbf{P_{G_k}}$ becomes $\mathbf{P_k}$ and D_g becomes $D = d^k$, which means that systematic grab sampling and systematic primary increment sampling methods become identical.

3. Comparison of the four sampling approaches

In order to compare the four sampling methods, we assume that the same analytical testing protocol will be followed irrespective of the method of sampling. For example, detection of *Salmonella* is based on incubation of the sampled material (grab or otherwise).

For detection of *Salmonella* in milk powder intended for general consumption, the International Organization for Standardization (ISO) recommends to gather 30 grab samples of 25g each forming a total sample amount of 750g; see ISO, 2017 (2017). Let us assume that the

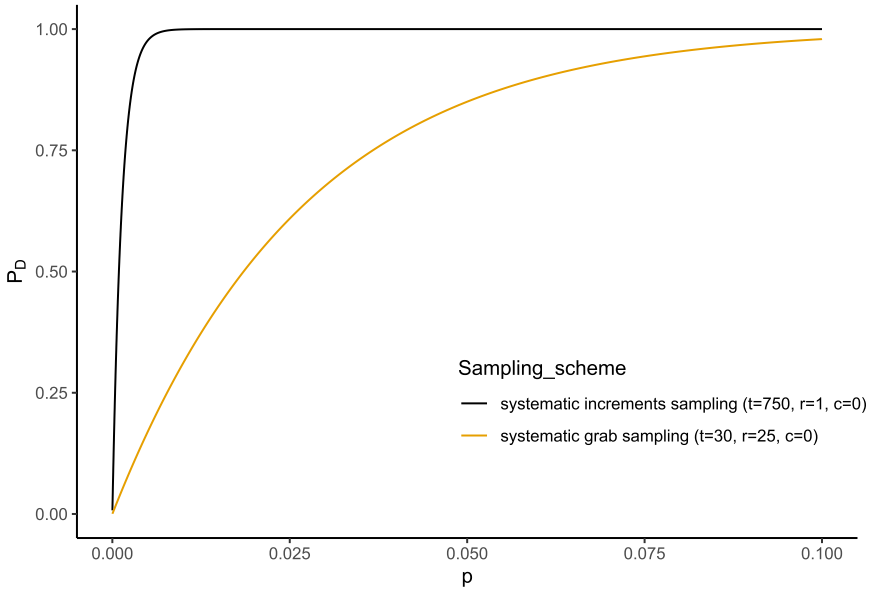

Fig. 1. Comparison of systematic grab sampling and systematic increments selection using autosamplers.

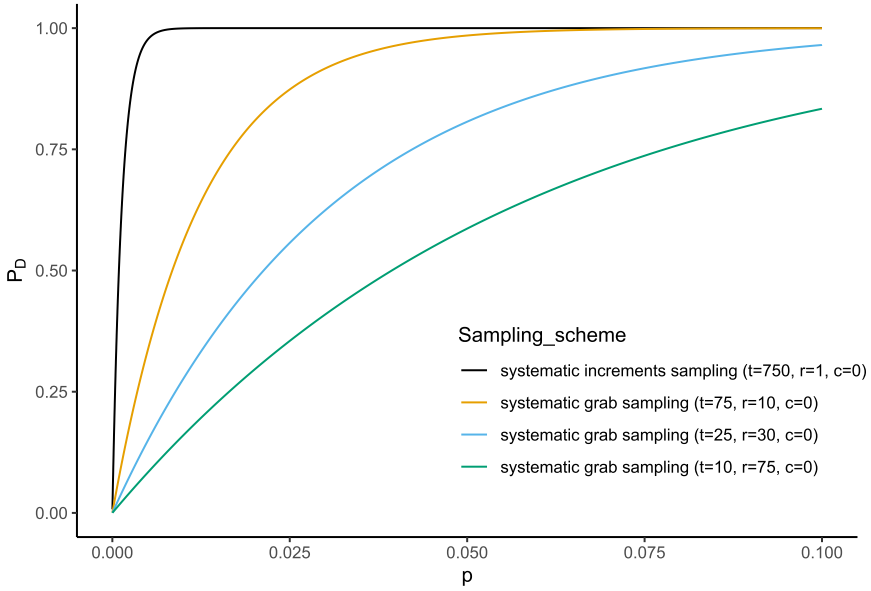

Fig. 2. The effect of number of systematic grab samples on probability of detection.

primary increment amount is 1 g of material (in order to be commensurate with the analytical sample amount for specific microorganism testing such as 10g for *Cronobacter* spp.). Let the batch quantity be $M = 10^7$g (or 10 metric tonnes) which are packaged in 400 bags of 25kg each. There is an obvious cost advantage in sampling the product during production before it is packaged, particularly using auto samplers. If 30 grab samples are to be taken after packaging the product, it requires the bags to be opened and hence such a method of sampling may not be economical for small batch sizes.

For the batch volume of $N = 10^7$, and sample size of $n = 750$ primary increments of 1g, Equations (3) and (6) produce almost identical probabilities of detection values because k is very large for large N and $d = 0.99$, which is graphically illustrated in Figure B8 of Appendix B. The value of d adopted here is realistic for *Salmonella* because its occurrence is rather rare; see Morlay et al. (2016). Other words, probability of contamination of the primary increment when it is absent in the previous increment is expected to be close to zero in *Salmonella* testing. On the other hand, contamination such as foreign matter or chemical in the milk powder would be more consistent with a less extreme d value such as 0.9 which can result in a small difference between systematic and random sampling of primary increments; see Qin et al. (2017). The likelihood of *Cronobacter* spp. (formerly called *Enterobacter sakazakii*) is higher than the likelihood of *Salmonella* or *Listeria* in milk powder. For such pathogens, a value of $d = 0.9$ may be adopted.

In other words, the systematic or random sampling of primary increments will involve the same risk of non-detection of *Salmonella* in milk powder for the total sampled amount of 750g. It is easier to configure robotic auto-samplers to draw systematic samples of primary increments and hence this strategy is desirable. Auto-samplers can also be configured to draw systematic grab samples of 25g instead of 1g primary increments and also detection probability can be calculated by using Equation (13). This strategy is not desirable because of the drop in probability of detection as illustrated in Fig. 1.

Fig. 2 compares the systematic grab sampling method for a total

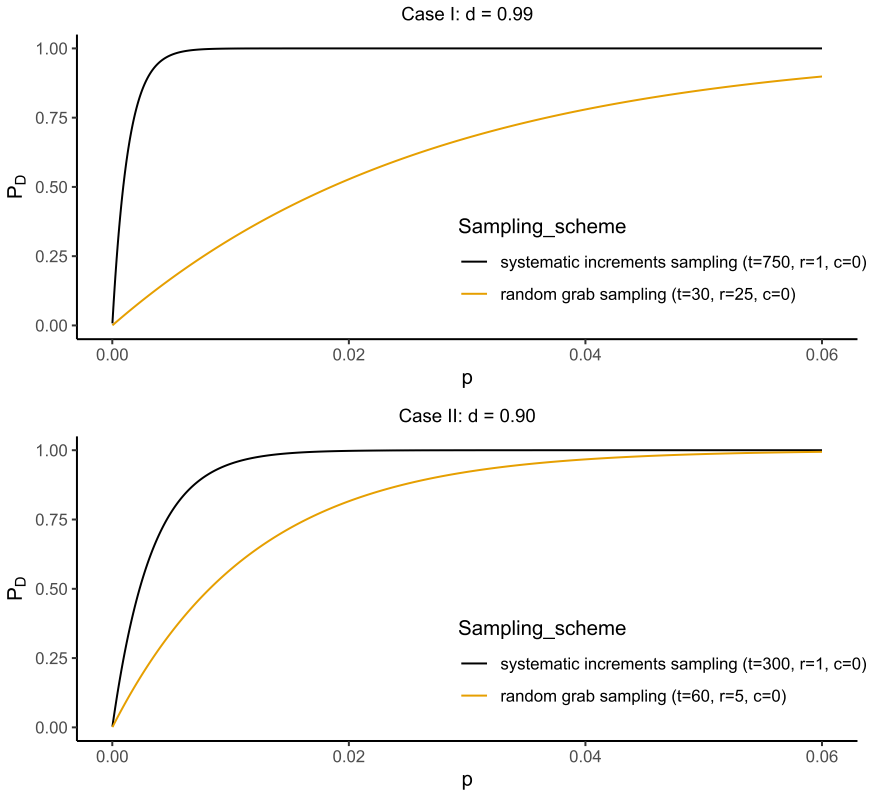

Fig. 3. Comparison of random grab sampling and systematic increments selection methods.

sample amount of 750g formed by different combinations of r and t. It is clear from this figure that drawing many systematic grab samples of smaller amount is a better strategy to improve detection when compared to drawing fewer grab samples of a more substantial amount. However the probability of detection for the grab sample method will still be inferior to the systematic autosampling of primary increments.

In the absence of auto-samplers, random grab sampling is the option commonly adopted. For $t = 30$ random grab samples and $r = 25$g, the probability of detection (of *Salmonella* in milk powder) remains poor when compared to systematic sampling of primary increments but at the same level of detection under systematic grab sampling. Testing for *Salmonella* is usually done using a subsample taken from the composite of the grab samples taken. Hence the probability of non-detection P_{ND} is the same as the probability of lot acceptance P_a (assuming that there are no false positive or negative errors). Fig. 3 (Case I) shows the P_D under random grab sampling and systematic increments selection methods for various p and given $t = 30$ and $r = 25$g.

The detection capability of the grab sampling method is improved with the increase in the number of grab samples taken as well as sample amount. Assume that 30 grab samples of 10g are taken for the detection of *Cronobacter* spp. in milk powder. These grab samples are often treated as random samples for risk modelling. Even though 60 grab samples of

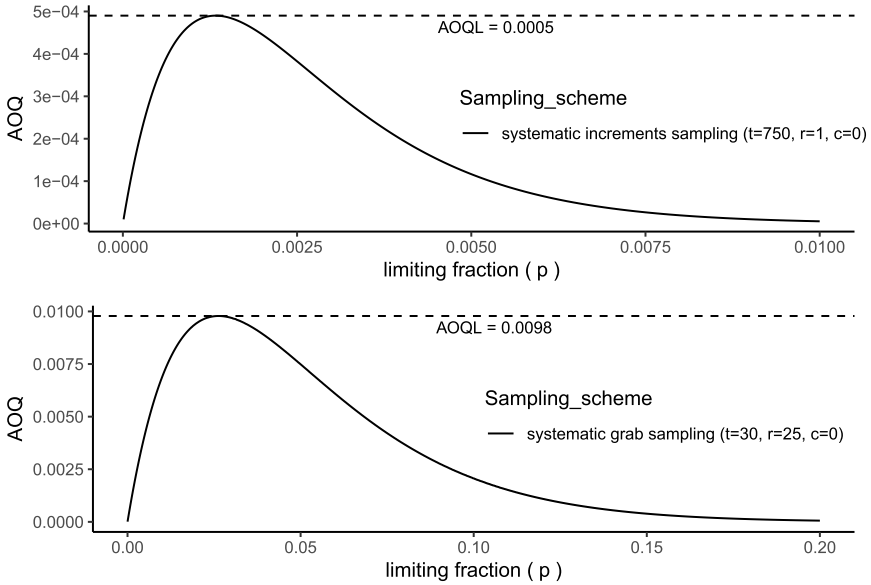

Fig. 4. Average outgoing quality (AOQ) versus p for sampling methods with.$d = 0.99$

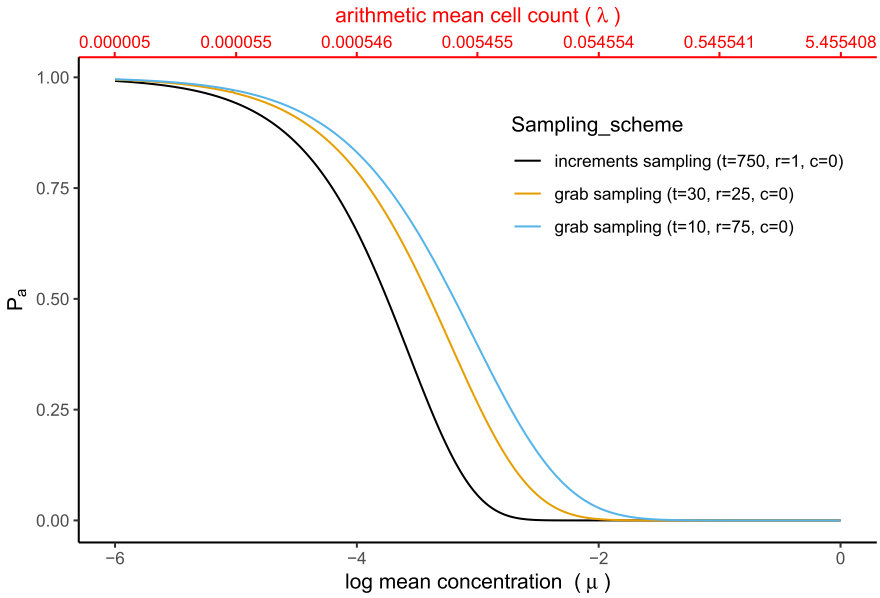

Fig. 5. Operating Characteristic (OC) curves of the sampling methods based on Poisson lognormal distribution with $\sigma_z = 0.8$.

5g ensure better detection when compared to 30 grab samples of 10g, they still fall short of the detection under systematic and random sampling from the process as seen from Fig. 3 (Case II).

The sampling methods employed for the detection plans can also be compared for their outgoing quality (OQ) performance. Only batches that pass the detection tests are cleared for customers. Since P_{ND} is the probability of non-detection, the outgoing contaminated proportion of primary increments is given by the product pP_{ND}; see McShane and Turnbull (1991). The quantity $AOQL$ is defined as the maximum proportion of outgoing contaminated primary increments and is given by

$$AOQL = \max_{0\le p\le 1} pP_{\mathrm{ND}} \tag{14}$$

We plotted AOQ for two different sampling schemes: 750 of 1g samples and 30 of 25g samples, as displayed in Fig. 4. The average outgoing quality limits of contaminated primary increments for the two sampling schemes are approximately 0.05% and 0.98% nonconforming respectively. Furthermore, systematic increments sampling achieves an AOQL of 0.05%, assuring that the worst fraction nonconforming the consumer receives as a long-term average is no more than 0.05%. Therefore, primary increment sampling, or in general, sampling small amounts more frequently, is more effective than the less frequent grab sampling method for protecting the consumer.

4. Further operating characteristic properties

Single sampling plan by attributes is the most commonly employed sampling inspection plan. The cumulative binomial distribution function gives the probability of acceptance:

$$P_a = \sum_{x=0}^{c} \binom{n}{x} p^x (1-p)^{n-x} \tag{15}$$

where P_a is the probability of acceptance, p is the proportion of contaminated increments, $\binom{n}{x}$ is the binomial coefficient, n is the number of primary increments in selected samples, c is the acceptance number and x is the number of contaminated increments. For the presence-absence testing for detection of food contamination, particularly pathogens, the acceptance number is generally zero ($c = 0$), so the probability of acceptance becomes

$$P_a = (1-p)^n \tag{16}$$

For risk evaluation in terms of microbial counts, the Operating Characteristic (OC) curve which plots the probability of acceptance against the underling concentration level is useful. Poisson mixture distributions are commonly employed for modelling the underlying microbial counts in the literature. Schothorst et al. (2009) and Gonzales-Barron and Butler (2011a) suggested that the Poisson-lognormal and Poisson-gamma distributions are particularly suitable for high and low microbial concentrations respectively.

Let Y be the random variable representing the count of microorganisms in a primary increment and m be the microbiological limit, then the probability of detection in a single primary increment is given by $p_d = P(Y > m)$. We can then compute the probability of acceptance in t samples as single plan by attribute which can be calculated from Equation (15). It is known that $E(Y)$, the arithmetic mean of the cell counts, is equal to $10^{\mu+0.5\,\ln(10)\sigma^2}$; see Mussida, Vose, and Butler (2013).

Let Z be the total count of microorganisms in the grab sample. Following Mussida, Vose, and Butler (2013), the count Z is nothing but the sum of identically distributed Poisson-lognormal random variables Y, thus the distribution of Z is also approximately Poisson-lognormal with mean μ_z, standard deviation σ_z where $E(Z) = rE(Y)$. The Poisson-lognormal distribution is appropriate when the number of microorganisms follows a Poisson distribution with rate λ which is lognormally distributed. Then the probability mass function in terms of log mean concentration μ_z and standard deviation σ_z is given by,

$$P(Z = z|\mu_z, \sigma_z) = \int_0^\infty P(z|\lambda) f(\lambda|\mu_z, \sigma_z) d\lambda \tag{17}$$

where the parameter μ_z, as the average count of microorganisms in the grab sample, can be estimated (assuming a fixed value of σ_z) by

$$\mu_z = \log_{10}(\lambda r) - \frac{\sigma_z^2}{2}\ln(10), \tag{18}$$

see Mussida, Vose, and Butler (2013).

The probability of detection in a primary increment is given by $p_d = 1 - P(Z = 0|\mu_z, \sigma_z)$ and so if we select t samples with zero acceptance sampling plan, the probability of acceptance is given by $P_a = (1-p_d)^t$.

In this paper, we fixed $\sigma_z = 0.8$ following Gonzales-Barron et al. (2013, p. 370), Jongenburger et al. (2015, p. 490) and others for the Poisson-lognormal case; see Dahms (2004), Schothorst et al. (2009),

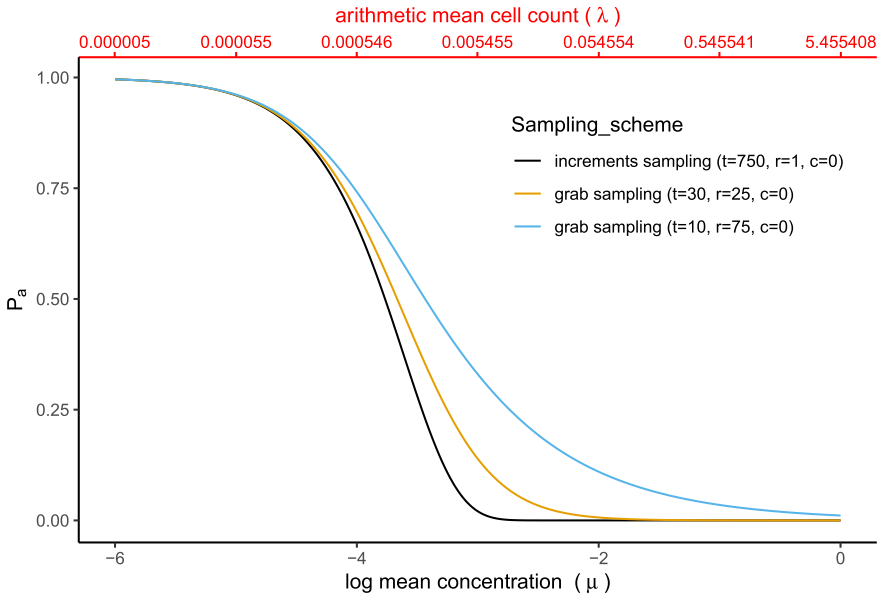

Fig. 6. Operating Characteristic (OC) curves of the sampling methods based on Poisson gamma distribution with $K = 0.05$.

Mussida, Vose, and Butler (2013) and Powell (2015). However, an OC curve can be constructed for different standard deviations as well. OC curves with different standard deviations such as $\sigma_z = 0.2, 0.4$ and 0.8 are also shown in Fig B9 of Appendix B. From this, it can be seen that the OC curve becomes flat for large standard deviations.

The Poisson gamma distribution is another suitable mixture distribution for food safety management, and whose probability mass function in terms of arithmetic mean of the cell counts λ and dispersion parameter K is given by,

$$P(Z=z|K,\lambda,r)=\frac{\Gamma(z+K)}{\Gamma(K)z!}\left(\frac{K}{K+\lambda r}\right)^{K}\left(\frac{\lambda r}{K+\lambda r}\right)^{z} \tag{19}$$

where Γ is the gamma function. If r primary increments form the total quantity of the sample, the probability of detection is given by

$$p_d=1-P(Z=0|K,\lambda,r)=1-\left(\frac{K}{K+\lambda r}\right)^{K} \tag{20}$$

If t samples are tested under a single sampling plan with zero acceptance number, the probability of acceptance is given by $P_a = (1-p_d)^t$. Following Gonzales-Barron and Butler (2011b), the dispersion parameter K for the Poisson-gamma case can be fixed in the range 0.044 and 0.401 and we used $K = 0.05$ for illustrative purposes; see Mussida, Gonzales-Barron, and Butler (2013).

Figs. 5 and 6 show the design effect of various sampling schemes on the probability of acceptance for various contamination levels. It is clear that drawing 750 samples of 1 g increments provides superior protection to drawing the same total weight such as 30 samples of 25g or 10 samples of 75g each.

Another way to monitor the risk is to examine the outgoing quality (OQ) performance as a function of the process microbial count. Only batches that pass the inspection are cleared for customers. Since P_a is the probability of acceptance, λ is the arithmetic mean of the cell count and the outgoing contaminated arithmetic mean of cell count of primary increments is given by AOQ as the product λP_a which is slightly different

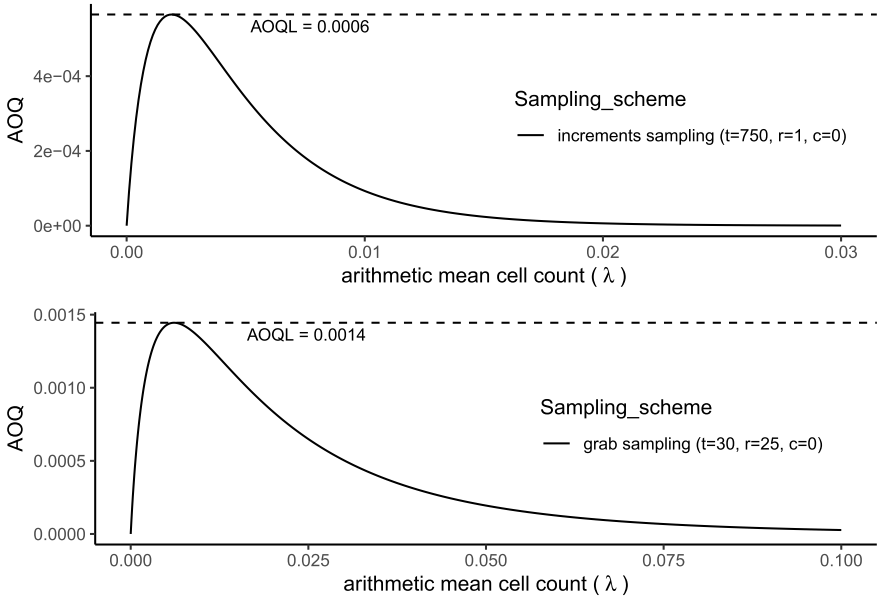

Fig. 7. Average outgoing quality (AOQ) versus arithmetic mean of cell count (λ) for sampling methods based on Poisson lognormal distribution with $\sigma_z = 0.8$.

to the classical *AOQ* formula. The quantity *AOQL* is defined as the maximum of outgoing contaminated primary increments and is given by

$$AOQL = \max_{\lambda \geq 0} \lambda P_a \tag{21}$$

The *AOQL* limits of contaminated primary increments for the two sampling schemes such as 750 samples of 1g increments and 30 samples of 25g subsamples each are approximately 0.06% and 0.14% non-conforming respectively. These limits of outgoing quality mirror the conclusion reached with the presence-absence testing based outgoing quality in 750g sampled as shown in Figs. 4 and 7. Therefore, we can conclude that sampling primary increments is more effective than grab sampling, resulting in higher protection to consumers.

5. R package "grabsampling"

We developed an *R* (R Core Team, 2020) software package *grabsampling* (available at https://github.com/Mayooran1987/grabsampling) for the probability of detection calculation for systematic or random grab sampling using a two-state Markov chain model. This package also draws the OC curves under various methods of sampling so that the efficacy of grab sampling for a different set of parameters can be assessed. The user can specify the parameters of the single sampling plan n and c. The package also allows for $c > 0$ even though the examples covered here are mainly based on $c = 0$. Description of our new package functions is available at https://mayooran1987.github.io/grabsampling.

6. Conclusion

This theoretical study has scrutinised the risk of non-detection when grab samples are employed, comparing it with the statistical 'gold standard' method of randomly sampling primary increments. Our approach allows for correlation of contamination in primary increments and the probability calculation is based on a two-state Markov chain. It was shown that the grab sampling method has a higher probability of non-detection when compared to sampling primary increments directly. We also presented a brief evaluation based on the OC and AOQ curves. The grab sampling methods exhibited enhanced risk of non-detection in general. So additional sampling is needed when grab samples are used for lot disposition when compared to direct sampling of the product from the process, with auto-samplers.

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Appendix A. Mathematical proofs

1. The transition probability matrix between blocks ($\mathbf{P_G}$).

$$P(\text{ND in block } (i+1) | \text{ND in block } i) = \frac{P(\text{ND in block } (i+1),\ \text{ND in block } i)}{P(\text{ND in block } i)} = \frac{(1-p)(1-a)^{2r-1}}{(1-p)(1-a)^{r-1}} = (1-a)^r = (1-p(1-d))^r = 1-a^*(\text{say})$$

$$P(\text{ND in block } (i+1) | \text{D in block } i) = \frac{P(\text{ND in block } (i+1),\ \text{D in block } i)}{P(\text{D in block } i)} = \frac{P(\text{ND in block } (i+1)) - P(\text{ND in block } (i+1),\ \text{ND in block } i)}{P(\text{D in block } i)}$$

$$= \frac{p_{nd} - (1-p)(1-a)^{2r-1}}{p_d} = \frac{p_{nd}(1-(1-a)^r)}{p_d} = \frac{a^* p_{nd}}{p_d} = b^*(\text{say})$$

Transition probability matrix between blocks is given by,

$$\mathbf{P_G} = \begin{matrix} \\ \text{ND} \\ \text{D} \end{matrix} \begin{matrix} \begin{matrix} \text{ND} & \text{D} \end{matrix} \\ \begin{bmatrix} 1-a^* & a^* \\ b^* & a^* \end{bmatrix} \end{matrix} = \begin{matrix} \\ \text{ND} \\ \text{D} \end{matrix} \begin{matrix} \begin{matrix} \text{ND} & \text{D} \end{matrix} \\ \begin{bmatrix} 1-(1-d_g)p_d & (1-d_g)p_d \\ (1-p_d)(1-d_g) & p_d + (1-p_d)d_g \end{bmatrix} \end{matrix}$$

where $a^* = 1-(1-p(1-d))^r$, $b^* = a^* p_{nd}/p_d$, a^* is the probability of contaminated presence in the block when it is absent in the previous block and serial correlation between blocks is $d_g = 1-a^*-b^*$.

2. Serial correlation between blocks.

$$d_g = 1-a^*-b^* = 1-\frac{a^*}{p_d} = 1-\frac{1-(1-p(1-d))^r}{p_d} = \frac{(1-p(1-d))^r - (1-p)(1-p(1-d))^{r-1}}{p_d} = \frac{dp(1-p(1-d))^{r-1}}{p_d}$$

Therefore,

$$d_g = \frac{dp(1-p(1-d))^{r-1}}{\left[1-(1-p)(1-p(1-d))^{r-1}\right]}$$

3. Probability of detection for systematic selection of grab

$$P(\text{non} - \text{detection in } t \text{ number of selected grab samples}) = P(\text{ND in block } 1, \text{ND in block } 2, \cdots, \text{ND in block } t) = P(\text{ND in block } 1)$$

$P(\text{ND in block } 2|\text{ND in block } 1)P(\text{ND in block } 3|\text{ND in block } 1, \text{ND in block } 2)$ $\cdots\cdots P(\text{ND in block } t|\text{ND in block } 1, \text{ND in block } 2 \ldots \text{ND in block } (t-1))$

By the Markov property, $= P(\text{ND in block } 1)\ P(\text{ND in block } 2|\text{ND in block } 1)P(\text{ND in block } 3|\text{ND in block } 2)\cdots\cdots P(\text{ND in block } t|\text{ND in block } (t-1))$

$$= p_{nd}(1-E)(1-E)\cdots\cdots(1-E) = p_{nd}(1-E)^{t-1} = p_{nd}\left[\left(1-p_d\left(1-d_g^k\right)\right)\right]^{t-1}$$

Therefore, the detection probability of all of the selected grab samples is given by,

$$P_{\text{D}} = 1-(1-p_d)\left[\left(1-p_d\left(1-d_g^k\right)\right)\right]^{t-1}$$

where $k = [N/rt]$.

For the probability of detection in all selected systematic auto-samples, fix $p_d = p$, $d_g = d$ and $t = n$. Therefore, the probability of detection in all selected systematic auto-samples is given by,

$$P_{\mathrm{D}} = 1 - (1-p)\left[\left(1 - p\left(1 - d^{k}\right)\right)\right]^{n-1}$$

Appendix B. Additional graphical displays

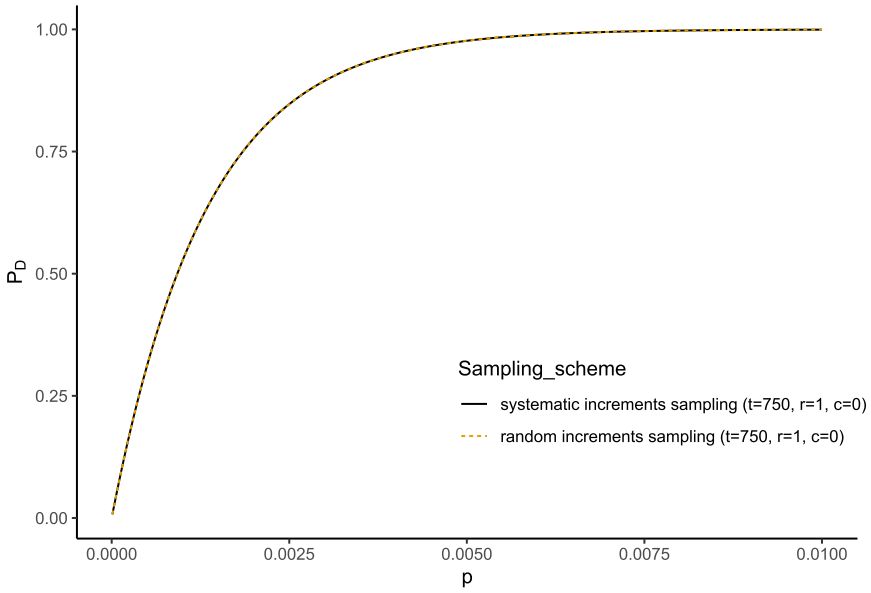

Figure B8. Comparison of systematic and random primary increments selection sampling.

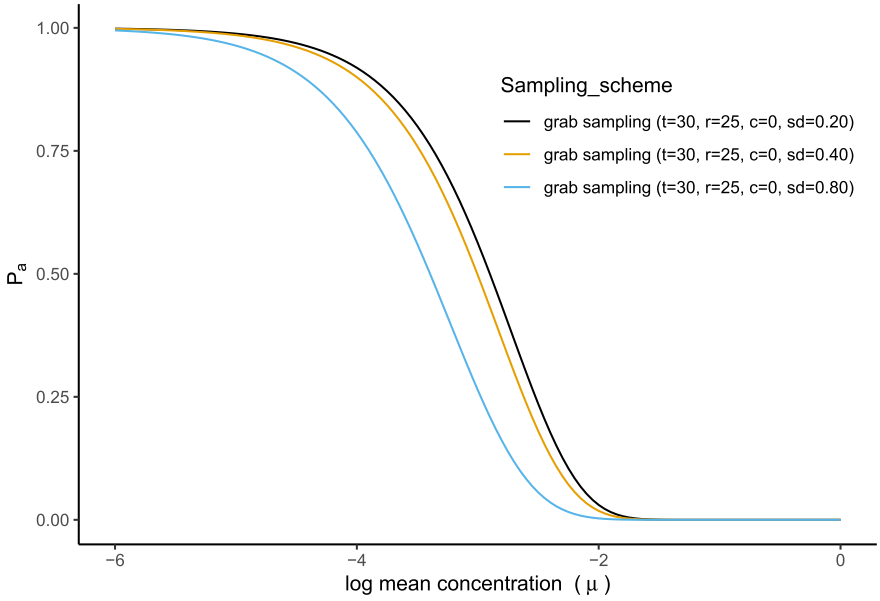

Figure B.9. Comparison of Operating Characteristic (OC) curves based on Poisson lognormal distribution with.$\sigma_z = 0.2, 0.4, 0.8$.

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